



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 3, 2020 – 08:53 pm BST

PDB ID : 6BZ8
Title : Thermus thermophilus 70S containing 16S G347U point mutation and near-cognate ASL Leucine in A site
Authors : Hoffer, E.D.; Maehigashi, T.; Fagan, C.E.; Dunham, C.M.
Deposited on : 2017-12-22
Resolution : 3.74 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

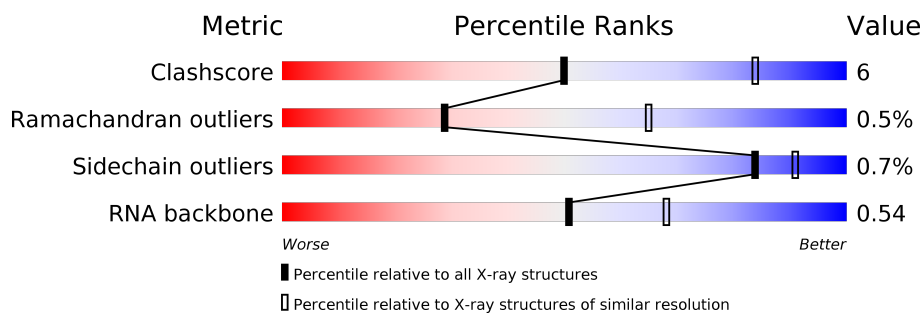
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.74 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1063 (3.90-3.58)
Ramachandran outliers	138981	1027 (3.90-3.58)
Sidechain outliers	138945	1023 (3.90-3.58)
RNA backbone	3102	1028 (4.46-3.00)

















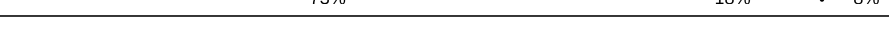

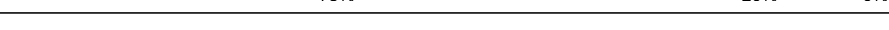
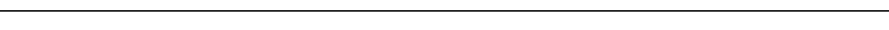
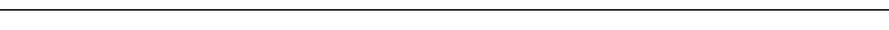
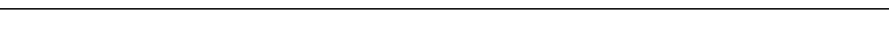
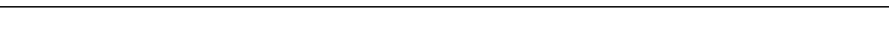
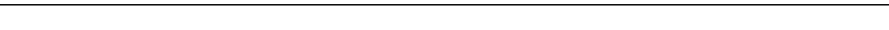

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	QA	1508	54% 36% 8% ..
1	XA	1508	54% 35% 8% ..
2	QB	256	70% 21% 8%
2	XB	256	74% 18% 8%
3	QC	239	75% 11% 14%
3	XC	239	76% 10% 14%
4	QD	209	80% 19%

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Mol	Chain	Length	Quality of chain
4	XD	209	 81% 18%
5	QE	162	 81% 12% 7%
5	XE	162	 80% 14% 7%
6	QF	101	 83% 17%
6	XF	101	 85% 15%
7	QG	156	 88% 11% .
7	XG	156	 86% 13% .
8	QH	138	 82% 17% .
8	XH	138	 82% 17% .
9	QI	128	 77% 21% ..
9	XI	128	 72% 26% ..
10	QJ	105	 69% 26% 6%
10	XJ	105	 69% 23% 9%
11	QK	129	 73% 19% 8%
11	XK	129	 73% 17% 10%
12	QL	132	 78% 16% . 5%
12	XL	132	 73% 18% . 8%
13	QM	126	 73% 21% . 5%
13	XM	126	 75% 20% 6%
14	QN	61	 82% 15% ..
14	XN	61	 85% 11% ..
15	QO	89	 93% 6% .
15	XO	89	 84% 13% .
16	QP	88	 82% 13% . 5%
16	XP	88	 83% 11% . 5%


























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Mol	Chain	Length	Quality of chain
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	QW	77	
22	XV	77	
22	XW	77	
23	QX	25	
23	XX	25	
24	QY	17	
24	XY	17	
25	RA	2915	
25	YA	2915	
26	RB	122	
26	YB	122	
27	RD	276	
27	YD	276	
28	RE	206	


























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Mol	Chain	Length	Quality of chain
28	YE	206	 75% 24%
29	RF	210	 79% 17% .
29	YF	210	 81% 15% .
30	RG	182	 76% 22% ..
30	YG	182	 73% 25% ..
31	RH	180	 76% 19% . .
31	YH	180	 76% 18% . . .
32	RI	148	 82% 16% ..
32	YI	148	 82% 16% ..
33	RN	140	 87% 11% .
33	YN	140	 88% 11% .
34	RO	122	 79% 20% .
34	YO	122	 80% 19% .
35	RP	150	 79% 21% .
35	YP	150	 78% 19% ..
36	RQ	141	 73% 27%
36	YQ	141	 74% 26%
37	RR	118	 79% 20% .
37	YR	118	 85% 14% .
38	RS	112	 78% 21% ..
38	YS	112	 76% 22% ..
39	RT	146	 74% 18% .. 6%
39	YT	146	 71% 22% .. 6%
40	RU	118	 76% 20% . .
40	YU	118	 77% 19% . .






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Mol	Chain	Length	Quality of chain
41	RV	101	
41	YV	101	
42	RW	113	
42	YW	113	
43	RX	96	
43	YX	96	
44	RY	110	
44	YY	110	
45	RZ	206	
45	YZ	206	
46	R0	85	
46	Y0	85	
47	R1	98	
47	Y1	98	
48	R2	72	
48	Y2	72	
49	R3	60	
49	Y3	60	
50	R4	71	
50	Y4	71	
51	R5	60	
51	Y5	60	
52	R6	54	
52	Y6	54	
53	R7	49	

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Mol	Chain	Length	Quality of chain
53	Y7	49	 86% 12% •
54	R8	65	 78% 15% 5% •
54	Y8	65	 80% 14% 5% •
55	R9	37	 84% 16%
55	Y9	37	 78% 22%

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 295646 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QA	1500	Total	C	N	O	P	0	0	0
			32244	14352	5978	10415	1499			
1	XA	1500	Total	C	N	O	P	0	0	0
			32246	14353	5981	10413	1499			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
QA	347	U	G	engineered mutation	GB 55771382
XA	347	U	G	engineered mutation	GB 55771382

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	QB	235	Total	C	N	O	S	0	0	0
			1907	1217	342	343	5			
2	XB	236	Total	C	N	O	S	0	0	0
			1915	1223	343	344	5			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	QC	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			
3	XC	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	QD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	XD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	QE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			
5	XE	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	QF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	XF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	QG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	XG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	QH	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			
8	XH	137	Total	C	N	O	S	0	0	0
			1108	700	214	192	2			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	QI	127	Total	C	N	O	0	0	0
			1010	639	197	174			
9	XI	126	Total	C	N	O	0	0	0
			998	633	193	172			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	QJ	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			
10	XJ	96	Total	C	N	O	S	0	0	0
			777	487	153	136	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	QK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	XK	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	QL	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			
12	XL	122	Total	C	N	O	S	0	0	0
			956	603	193	159	1			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	QM	120	Total	C	N	O	S	0	0	0
			955	591	197	165	2			
13	XM	119	Total	C	N	O	S	0	0	0
			946	585	195	164	2			

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	QN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	XN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	QO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	XO	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	QP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			
16	XP	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	QQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			
17	XQ	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	QR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	XR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	83	Total	C	N	O	S	0	0	0
			665	424	124	115	2			
19	XS	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	QT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	XT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	QU	25	Total	C	N	O	0	0	0
			217	134	52	31			
21	XU	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 22 is a RNA chain called tRNA fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
22	QW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	XV	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			
22	XW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	8	Total	C	N	O	P	0	0	0
			167	75	27	57	8			
23	XX	11	Total	C	N	O	P	0	0	0
			230	105	42	73	10			

- Molecule 24 is a RNA chain called ASL Leu.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	17	Total	C	N	O	P	0	0	0
			362	162	65	118	17			
24	XY	17	Total	C	N	O	P	0	0	0
			362	162	65	118	17			

- Molecule 25 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	RA	2882	Total	C	N	O	P	0	0	0
			62071	27627	11611	19952	2881			
25	YA	2883	Total	C	N	O	P	0	0	0
			62091	27636	11613	19960	2882			

- Molecule 26 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	RB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			
26	YB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	RD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			
27	YD	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	RE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			
28	YE	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	RF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			
29	YF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	RG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	YG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	RH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			
31	YH	174	Total	C	N	O	S	0	0	0
			1336	848	251	236	1			

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	RI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			
32	YI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 33 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	RN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
33	YN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	RO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
34	YO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	RP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			
35	YP	147	Total	C	N	O	S	0	0	0
			1122	698	229	192	3			

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	RQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
36	YQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	RR	117	Total	C	N	O	0	0	0
			960	599	202	159			
37	YR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	RS	111	Total	C	N	O	0	0	0
			882	556	176	150			
38	YS	111	Total	C	N	O	0	0	0
			882	556	176	150			

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	RT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			
39	YT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 40 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	RU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
40	YU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 41 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	RV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
41	YV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 42 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	RW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			
42	YW	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	RX	92	Total	C	N	O		0	0	0
			725	471	131	123				
43	YX	92	Total	C	N	O		0	0	0
			725	471	131	123				

- Molecule 44 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	RY	107	Total	C	N	O	S	0	0	0
			818	525	155	132	6			
44	YY	107	Total	C	N	O	S	0	0	0
			818	525	155	132	6			

- Molecule 45 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			
45	YZ	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	R0	81	Total	C	N	O	S	0	0	0
			643	398	137	107	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	Y0	75	Total	C	N	O	S	0	0	0
			599	370	127	101	1			

- Molecule 47 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	R1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			
47	Y1	93	Total	C	N	O	S	0	0	0
			729	457	145	126	1			

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	R2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			
48	Y2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	R3	59	Total	C	N	O	0	0	0
			469	298	90	81			
49	Y3	59	Total	C	N	O	0	0	0
			469	298	90	81			

- Molecule 50 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	R4	69	Total	C	N	O	S	0	0	0
			565	356	103	101	5			
50	Y4	69	Total	C	N	O	S	0	0	0
			565	356	103	101	5			

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	R5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
51	Y5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	R6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
52	Y6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	R7	47	Total	C	N	O	S	0	0	0
			409	251	102	54	2			
53	Y7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	R8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
54	Y8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	R9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
55	Y9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QA	72	Total	Mg	0	0
			72	72		
56	RP	2	Total	Mg	0	0
			2	2		
56	QX	1	Total	Mg	0	0
			1	1		
56	YA	541	Total	Mg	0	0
			541	541		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	Y5	1	Total 1	Mg 1	0	0
56	RT	1	Total 1	Mg 1	0	0
56	RN	1	Total 1	Mg 1	0	0
56	XE	1	Total 1	Mg 1	0	0
56	XS	1	Total 1	Mg 1	0	0
56	YD	1	Total 1	Mg 1	0	0
56	XX	1	Total 1	Mg 1	0	0
56	QV	6	Total 6	Mg 6	0	0
56	Y8	1	Total 1	Mg 1	0	0
56	YO	1	Total 1	Mg 1	0	0
56	XA	80	Total 80	Mg 80	0	0
56	YY	1	Total 1	Mg 1	0	0
56	RQ	2	Total 2	Mg 2	0	0
56	R0	3	Total 3	Mg 3	0	0
56	RO	1	Total 1	Mg 1	0	0
56	QH	1	Total 1	Mg 1	0	0
56	YQ	3	Total 3	Mg 3	0	0
56	RY	1	Total 1	Mg 1	0	0
56	QC	1	Total 1	Mg 1	0	0
56	R8	1	Total 1	Mg 1	0	0
56	YX	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	RR	2	Total 2	Mg 2	0	0
56	Y7	1	Total 1	Mg 1	0	0
56	QF	1	Total 1	Mg 1	0	0
56	Y0	2	Total 2	Mg 2	0	0
56	XQ	1	Total 1	Mg 1	0	0
56	RA	513	Total 513	Mg 513	0	0
56	YP	4	Total 4	Mg 4	0	0
56	RE	3	Total 3	Mg 3	0	0
56	XL	1	Total 1	Mg 1	0	0
56	YB	12	Total 12	Mg 12	0	0
56	XC	1	Total 1	Mg 1	0	0
56	QY	1	Total 1	Mg 1	0	0
56	XV	8	Total 8	Mg 8	0	0
56	RB	11	Total 11	Mg 11	0	0
56	XM	1	Total 1	Mg 1	0	0
56	YE	3	Total 3	Mg 3	0	0

- Molecule 57 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
57	QD	1	Total	Fe	S	0	0
			8	4	4		
57	XD	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	Y9	1	Total	Zn	0	0
			1	1		
58	YY	1	Total	Zn	0	0
			1	1		
58	Y6	1	Total	Zn	0	0
			1	1		
58	QN	1	Total	Zn	0	0
			1	1		
58	XN	1	Total	Zn	0	0
			1	1		
58	RY	1	Total	Zn	0	0
			1	1		
58	Y4	1	Total	Zn	0	0
			1	1		
58	R6	1	Total	Zn	0	0
			1	1		
58	Y5	1	Total	Zn	0	0
			1	1		
58	R5	1	Total	Zn	0	0
			1	1		

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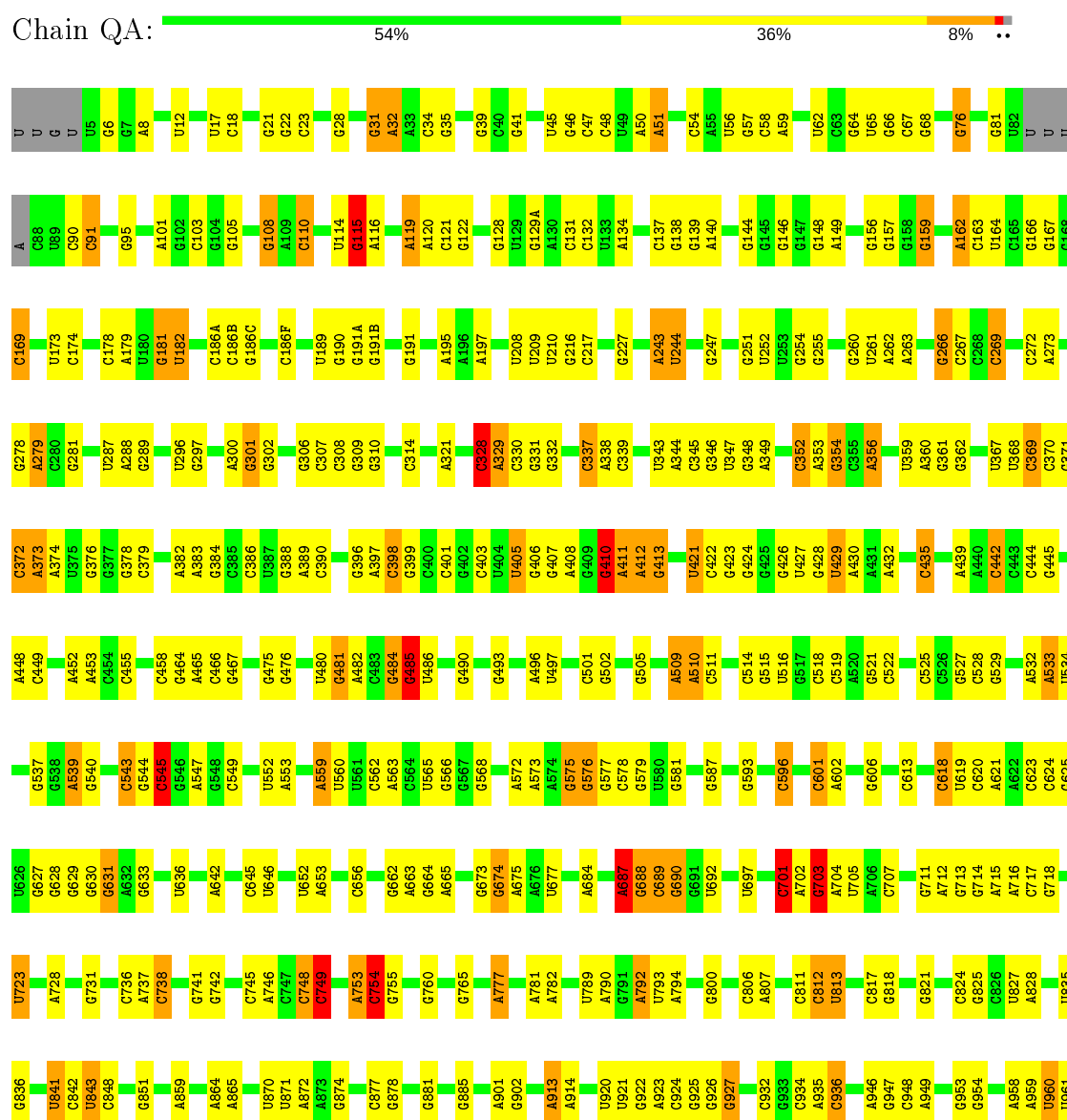
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	R4	1	Total 1	Zn 1	0	0
58	R9	1	Total 1	Zn 1	0	0

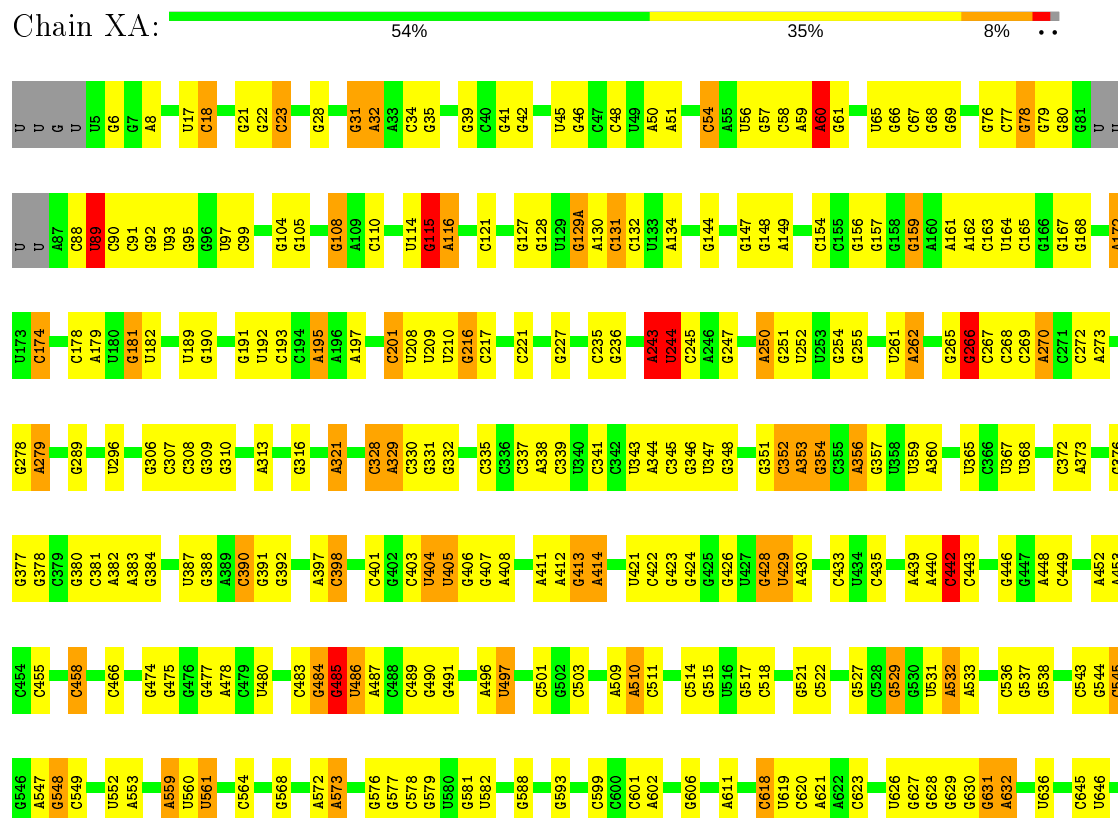
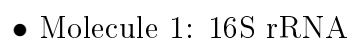
3 Residue-property plots [i](#)

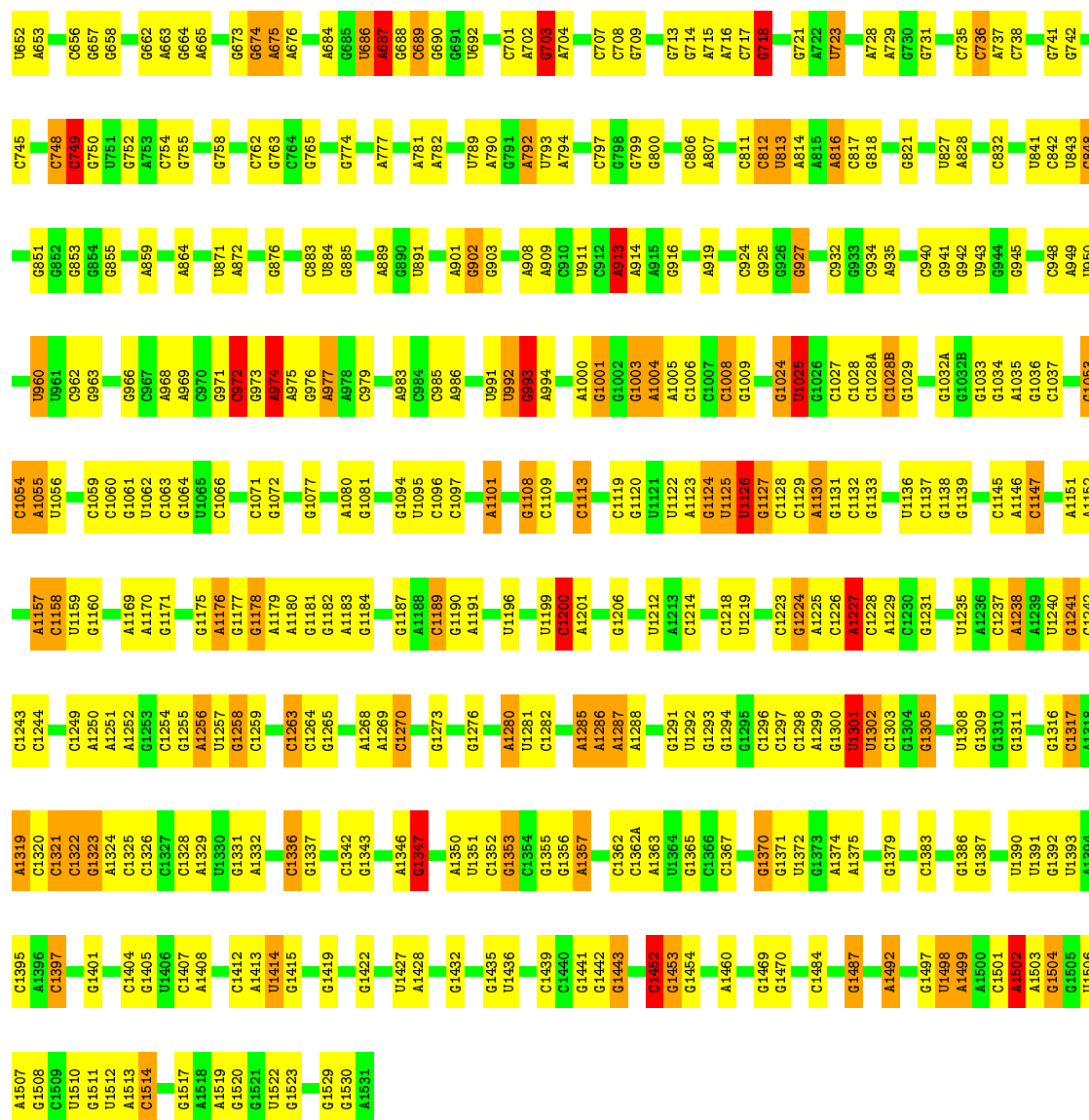
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

- Molecule 1: 16S rRNA

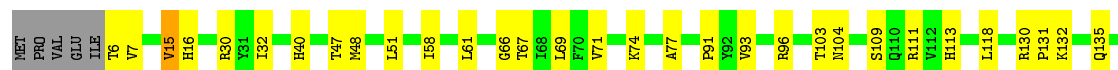






• Molecule 2: 30S ribosomal protein S2

Chain QB: 70% 21% 8%



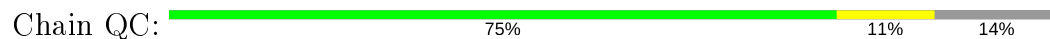
• Molecule 2: 30S ribosomal protein S2

Chain XB: 74% 18% 8%

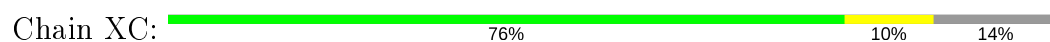




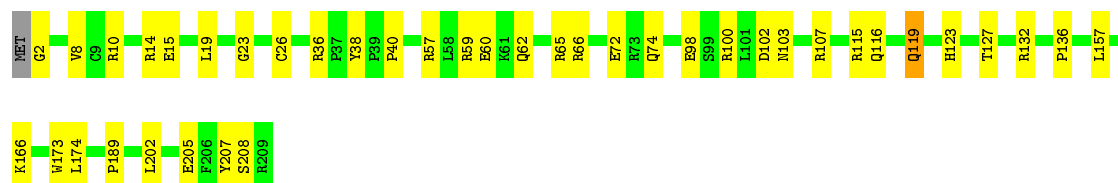
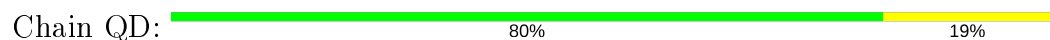
- Molecule 3: 30S ribosomal protein S3



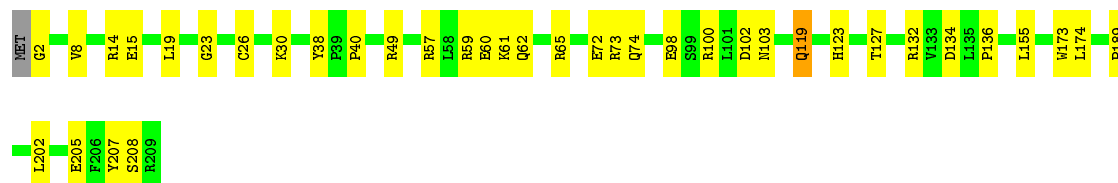
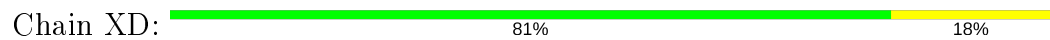
- Molecule 3: 30S ribosomal protein S3



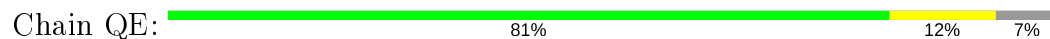
- Molecule 4: 30S ribosomal protein S4




- Molecule 4: 30S ribosomal protein S4

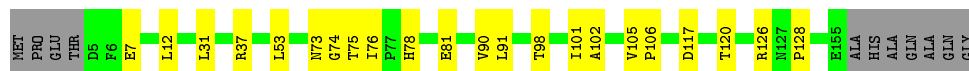


- Molecule 5: 30S ribosomal protein S5




- Molecule 5: 30S ribosomal protein S5

Chain XE:  80% 14% 7%




- Molecule 6: 30S ribosomal protein S6

Chain QF:  83% 17%



- Molecule 6: 30S ribosomal protein S6

Chain XF:  85% 15%




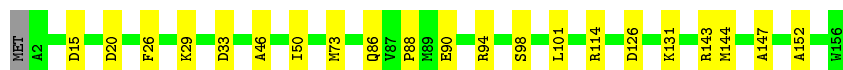
- Molecule 7: 30S ribosomal protein S7

Chain QG:  88% 11%




- Molecule 7: 30S ribosomal protein S7

Chain XG:  86% 13%




- Molecule 8: 30S ribosomal protein S8

Chain QH:  82% 17%




- Molecule 8: 30S ribosomal protein S8

Chain XH:  82% 17%



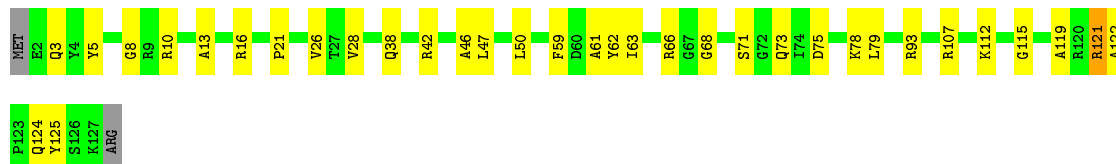
- Molecule 9: 30S ribosomal protein S9

Chain QI:  77% 21% ..



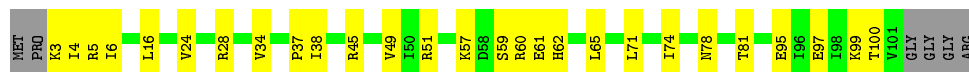
- Molecule 9: 30S ribosomal protein S9

Chain XI:  72% 26% ..



- Molecule 10: 30S ribosomal protein S10

Chain QJ:  69% 26% 6%



- Molecule 10: 30S ribosomal protein S10

Chain XJ:  69% 23% 9%



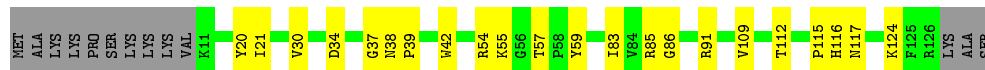
- Molecule 11: 30S ribosomal protein S11

Chain QK:  73% 19% 8%




- Molecule 11: 30S ribosomal protein S11

Chain XK:  73% 17% 10%



- Molecule 12: 30S ribosomal protein S12

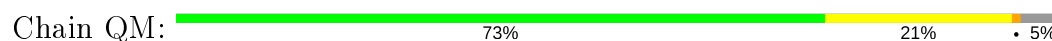
Chain QL:  78% 16% 5%



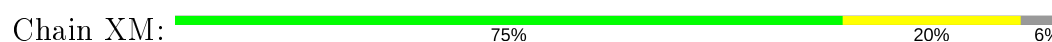
- Molecule 12: 30S ribosomal protein S12



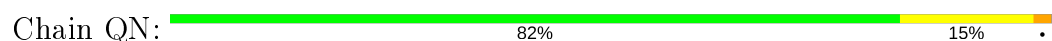
- Molecule 13: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14 type Z



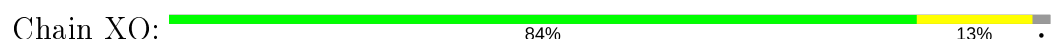
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 15: 30S ribosomal protein S15



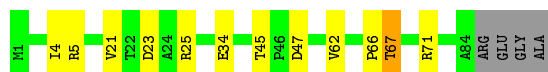
- Molecule 15: 30S ribosomal protein S15





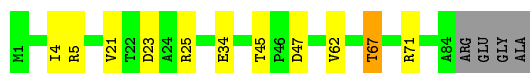
- Molecule 16: 30S ribosomal protein S16

Chain QP: 82% 13% 5%



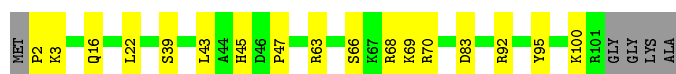
- Molecule 16: 30S ribosomal protein S16

Chain XP: 83% 11% 5%



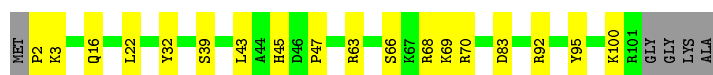
- Molecule 17: 30S ribosomal protein S17

Chain QQ: 79% 16% 5%



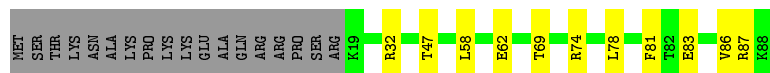
- Molecule 17: 30S ribosomal protein S17

Chain XQ: 78% 17% 5%



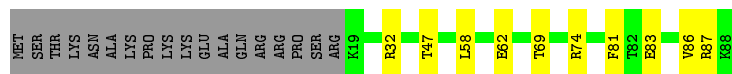
- Molecule 18: 30S ribosomal protein S18

Chain QR: 67% 13% 20%



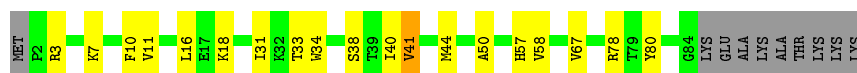
- Molecule 18: 30S ribosomal protein S18

Chain XR: 68% 11% 20%



- Molecule 19: 30S ribosomal protein S19

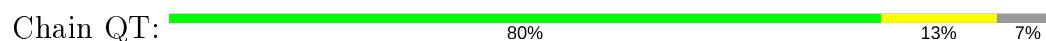
Chain QS: 69% 19% 11%



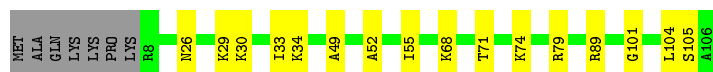
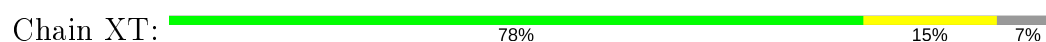
- Molecule 19: 30S ribosomal protein S19



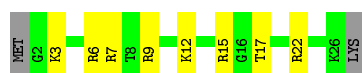
- Molecule 20: 30S ribosomal protein S20



- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein Thx



- Molecule 21: 30S ribosomal protein Thx

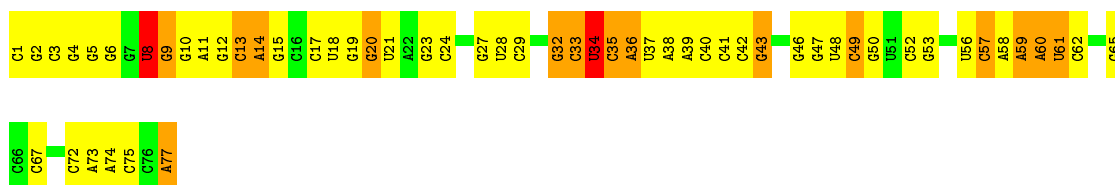


- Molecule 22: tRNA fMet



- Molecule 22: tRNA fMet





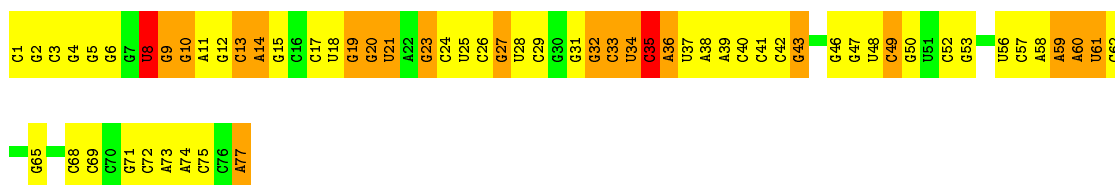
- Molecule 22: tRNA fMet

Chain XV: 61% 29% 8% .



- Molecule 22: tRNA fMet

Chain XW: 19% 53% 25% .



- Molecule 23: messenger RNA

Chain QX: 28% 68% .



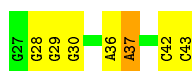
- Molecule 23: messenger RNA

Chain XX: 28% 8% 8% 56%



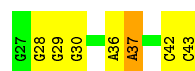
- Molecule 24: ASL Leu

Chain QY: 59% 35% 6%



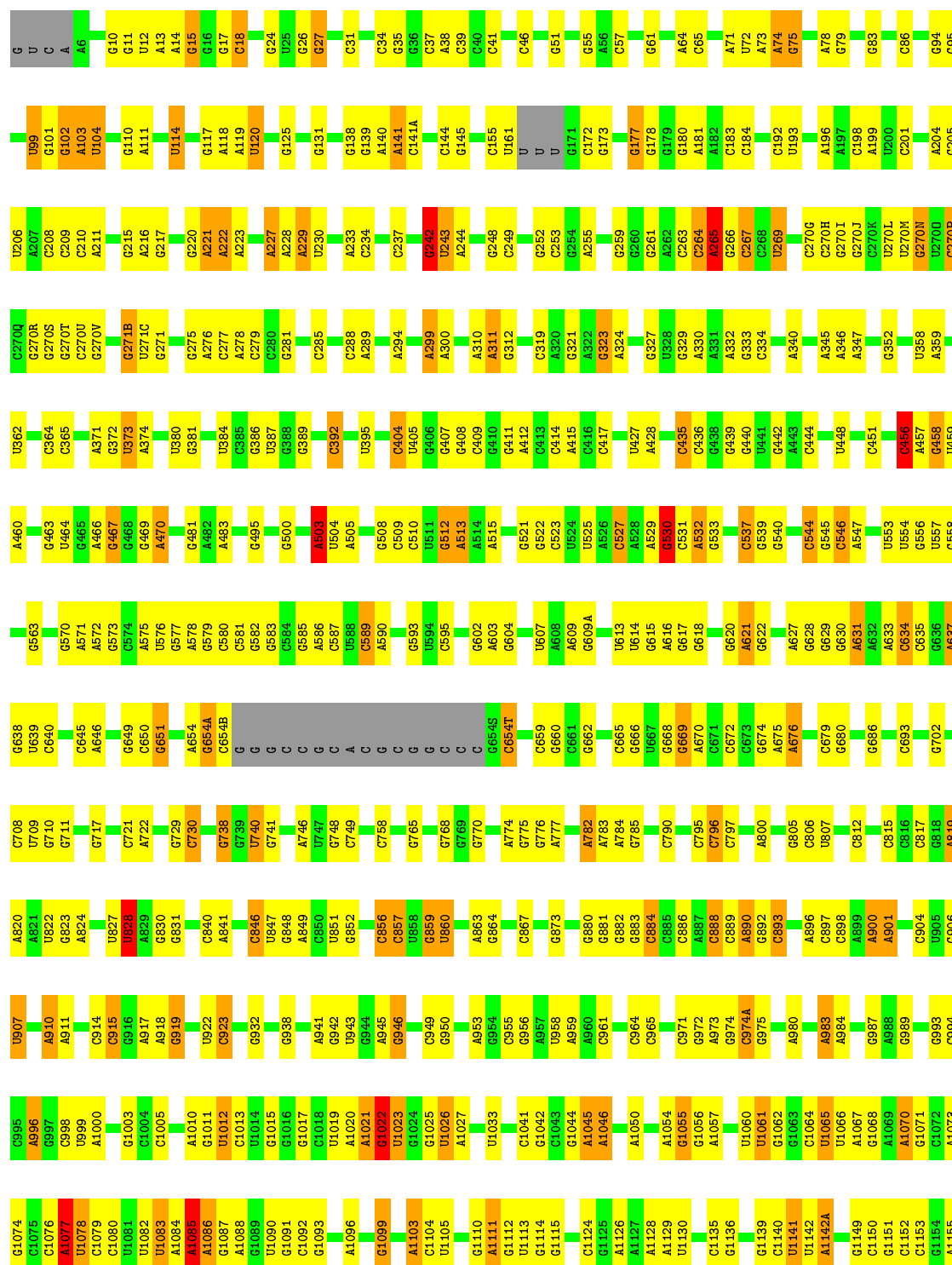
- Molecule 24: ASL Leu

Chain XY: 59% 35% 6%



• Molecule 25: 23S rRNA

Chain RA: 56% 34% 8% ..



A2542	G2444	G2341	U2249	U2150	C2063	A1847	G1764	C1644	C1547	C1458	G1371	U1267	A1156
G2543	G2445	C2342	G2250	G2152	C2064	U1851	C1771	C1648	C1548	G1459	U1372	G1270	G1157
U2547	A2448	G2345	C2254	G2156	C2065	C1852	G1772	G1649	C1549	G1460	C1376	G1271	U1165
G2553	C2456	A2346	C2258	G2157	U1963	A1853	A1773	G1650	C1549	G1461	G1377	A1272	U1166
U2554	C2456	C2347	C2258	G2158	U1964	G1858	C1774	G1651	A1554	C1462	A1378	A1273	G1170
C2556	C2461	C2350	A2286	A2158	C2069	U1859	U1775	A1652	A1558	A1471	A1379	U1288	G1171
C2559	C2467	G2354	A2289	C2161	C2073	A1860	G1776	C1656	A1559	A1472	G1380	U1288	A1173
C2560	C2468	A2289	A2289	G2162	U2074	G1869	U1779	C1657	A1560	A1473	G1385	U1294	A1174
A2561	A2469	G2358	A2273	C2163	U2075	C1870	C1781	U1659	A1566	G1474	G1385	C1295	G1176
U2562	C2470	A2361	A2274	C2164	A1970	C1871	C1782	C1660	A1567	U1479	U1391	G1296	A1177
C2566	C2471	C2361	C2275	G2166	A1972	A1872	A1783	G1661	A1568	A1482	A1392	C1297	C1178
A2566	C2474	C2368	A2278	U2167	G1973	G1878	A1784	C1662	A1569	U1483	C1393	C1298	C1179
C2567	C2475	A2169	G2087	G2168	C1979	C1881	A1786	C1663	U1578	U1484	A1394	G1299	C1180
C2568	C2374	A2170	G2087	A2170	C1979	C1882	A1786	A1664	A1579	G1485	A1395	U1300	G1184
G2569	C2374	A2170	G2087	A2170	C1979	C1882	A1786	A1664	A1579	G1485	A1395	U1300	G1184
G2570	A2378	A2173	C2283	A2173	C1990	G1883	A1789	G1666	C1582	A1486	G1398	G1309	G1187
C2571	G2379	C2284	C2284	U2096	U1991	A1884	A1790	C1670	A1583	A1487	C1399	U1312	G1191
A2572	C2380	C2285	C2285	U2102	U1992	A1885	A1791	G1674	C1585	A1490	G1401	U1313	G1191
G2573	C2383	C2286	C2286	C2103	U1993	G1888	C1795	C1675	A1586	U1491	G1402	C1314	G1195
C2574	A2384	A2287	A2287	C2104	C1995	A1889	U1796	C1675	A1587	C1493	C1403	C1315	C1202
G2575	G2384	A2288	A2288	G2105	C2006	C1893	U1797	G1678	C1588	A1494	C1404	U1316	G1203
G2576	C2385	C2187	C2187	C2106	C2006	C1893	U1798	U1679	C1589	U1497	U1405	A1317	G1204
A2577	U2387	G2190	C2292	G2107	G2010	A1901	G1799	U1679	A1590	C1504	U1406	C1318	A1204
C2579	C2387	C2190	C2292	C2107	U2011	C1902	C1800	C1686	A1591	C1509	C1407	G1319	U1205
G2494	A2392	G2193	C2293	U2109	G2012	G1903	A1801	C1686	C1592	A1510	C1417	C1320	G1206
G2495	C2393	C2194	U2296	G2110	A2013	A1904	A1803	A1689	G1594	C1506	G1418	A1322	A1210
A2496	C2394	C2195	U2296	C2111	C2019	C1905	C1804	C1689	G1595	A1507	G1419	A1323	U1211
C2497	C2395	U2197	G2299	C2112	A2020	G1913	A1809	C1694	C1599	A1508	U1420	G1330	C1230
C2498	C2396	A2198	C2303	U2113	G2023	C1914	A1810	G1695	C1600	C1514	G1421	A1331	G1231
C2499	C2396	A2199	C2303	G2114	G2023	U1915	A1811	A1698	C1600	C1515	G1422	C1332	G1232
U2500	C2402	A2200	G2307	G2115	A2030	C1920	A1812	G1703	C1605	U1520	G1423	G1334	G1236
A2503	C2403	C2205	C2308	A2117	A2031	U1920	A1815	G1703	G1606	G1526	A1427	U1341	A1237
U2504	U2406	G2210	C2308	A2118	A2032	C1920	G1816	G1725	G1607	G1527	C1428	A1349	G1238
G2505	U2406	G2211	A2311	A2119	G2032	A1927	G1817	G1725	A1608	A1528	C1430	A1241	A1241
U2506	G2410	A2212	U2312	G2123	U2034	A1928	U1818	G1728	A1609	U1516	U1433	A1352	A1247
C2507	G2410	U2213	C2314	G2124	G2035	G1929	A1819	A1729	A1610	U1520	U1433	A1353	A1247
G2508	G2421	G2215	C2315	G2125	G2035	G1930	U1820	U1730	C1611	U1520	C1437	A1354	A1247
C2512	A2422	A2225	C2315	A2126	U2041	U1931	A1824	G1733	A1614	G1526	A1427	A1359	A1253
G2513	U2423	C2226	G2319	G2127	A2042	A1936	G1825	G1733	A1615	G1527	C1428	A1359	A1254
U2514	C2424	A2227	A2320	C2128	C2043	A1937	G1826	G1741	A1616	A1528	C1430	A1352	U1255
C2515	A2426	G2228	G2321	G2129	U2047	A1938	C1827	G1742	A1617	U1533	U1433	A1353	G1256
G2516	C2427	U2132	C2325	G2130	G2048	U1939	G1828	G1743	A1618	C1534	C1445	A1354	G1256
C2517	G2428	U2133	C2326	G2131	G2048	U1940	A1829	G1743	A1619	U1534	C1445	A1354	A1262
A2518	G2429	G2133	C2327	A2134	G2052	C1947	C1830	C1751	G1622	U1535	C1445	A1359	A1263
U2519	A2435	A2135	A2328	A2136	C2056	U1947	U1833	G1752	G1622	A1536	A1444A	A1359	A1264
G2529	A2435	C2137	U2343	C2137	G2056	U1951	U1834	C1754	G1636	C1537	C1445	A1363	G1265
A2439	A2439	U2244	U2244	U2244	G2056	U1951	G1835	A1755	A1637	G1538	A1449	A1365	A1262
C2534	C2440	U2245	G2334	U2245	A2059	A1952	U1835	G1756	C1638	U1542	A1449	A1365	U1263
C2535	C2441	G2246	A2336	G2246	A2060	A1952	U1835	G1756	C1638	A1543	G1449A	A1368	U1263
C2536	C2442	A2247	A2336	A2247	G2061	U1955	C1844	G1762	C1639	A1544	U1454	G1369	A1265
A2541	C2443	G2248	C2248	G2149	A2062	U1956	G1846	G1763	C1640	A1545	G1455	C1370	G1266







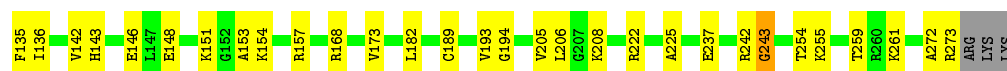
G81	G86	G87	G88	G89	A89A	A101	G105	G106	G107	G108	G109	G110	G111	G112	G118	A119	U	U																													
U1	C2	C3	C4	C5	U8	C11	C12	A13	U14	A15	G16	U22	G23	G24	A25	A26	G27	C30	C31	C32	G33	U34	U35	C36	C37	U41	C42	C43	G44	A45	A46	C47	A48	C49	A52	A53	G56	C60	G61	A66	G67	C70	A73	U74	G75	C79	U90

- Molecule 26: 5S rRNA

A89A	U1
	C2
A101	C3
	C4
G105	C5
G106	C6
U107	C7
C108	C8
G109	C9
G110	C10
U111	C11
G112	C12
C113	A13
G114	U14
G115	A15
G116	G16
G117	
G118	G22
A119	G23
U	G24
U	A25
	A26
	G27
	C28
	A29
	C30
	C31
	C32
	G33
	U34
	U35
	U41
	C42
	C43
	C44
	C45
	A46
	C47
	A53
	C60
	G61
	A66
	G67
	C70
	A73
	C79
	U80
	G81
	G86
	G87
	C88
	C89

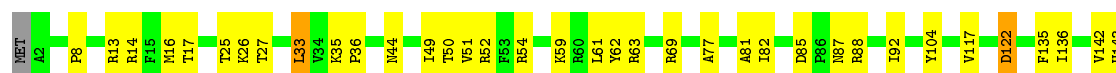
- Molecule 27: 50S ribosomal protein L2

Met	A2	P8	R13	R14	F15	M16	T17	I24	T25	K26	T27	L33	V34	K35	P36	M44	M45	Q46	I49	T50	V51	B52	F53	R54	L61	Y62	R63	R69	A77	A81	I82	D85	P86	N87	R88	R91	I92	D99	Y104	V117	P121	D122
-----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------



- Molecule 27: 50S ribosomal protein L2

Chain YD: 75% 22% ..



- Molecule 28: 50S ribosomal protein L3

Chain RE: 76% 23%



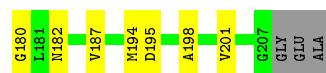
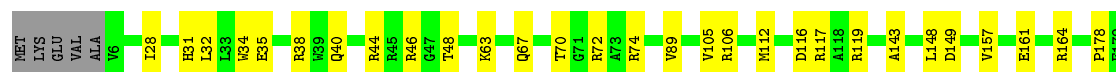
- Molecule 28: 50S ribosomal protein L3

Chain YE: 75% 24%



- Molecule 29: 50S ribosomal protein L4

Chain RF: 79% 17%



- Molecule 29: 50S ribosomal protein L4

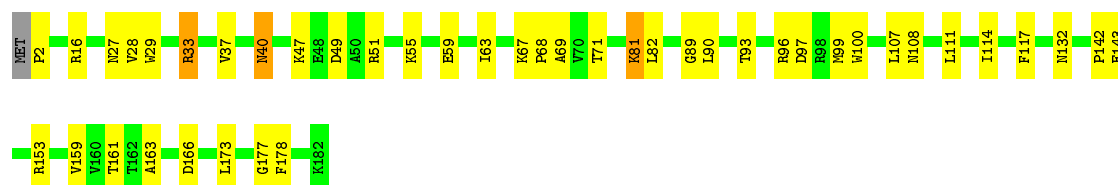
Chain YF: 81% 15%





- Molecule 30: 50S ribosomal protein L5

Chain RG: 76% 22% ..



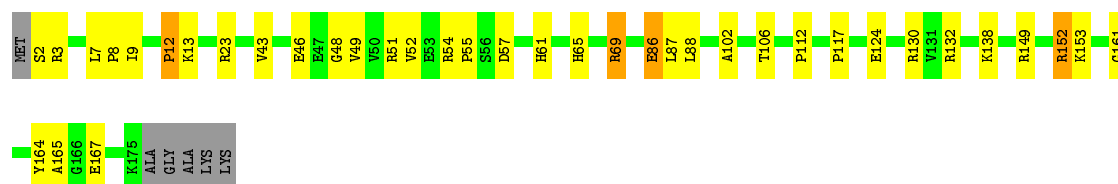
- Molecule 30: 50S ribosomal protein L5

Chain YG: 73% 25% ..



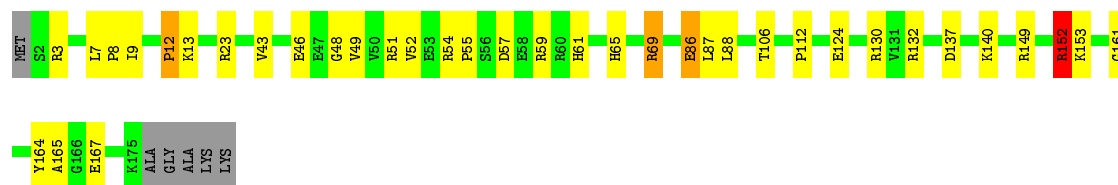
- Molecule 31: 50S ribosomal protein L6

Chain RH: 76% 19% ..



- Molecule 31: 50S ribosomal protein L6

Chain YH: 76% 18% ..




- Molecule 32: 50S ribosomal protein L9

Chain RI: 82% 16% ..



- Molecule 32: 50S ribosomal protein L9

Chain YI:  82% 16% ..



- Molecule 33: 50S ribosomal protein L13

Chain RN:  87% 11% .




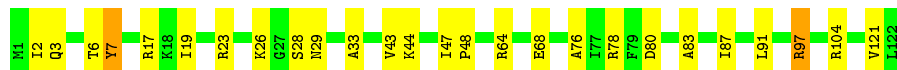
- Molecule 33: 50S ribosomal protein L13

Chain YN:  88% 11% .




- Molecule 34: 50S ribosomal protein L14

Chain RO:  79% 20% .




- Molecule 34: 50S ribosomal protein L14

Chain YO:  80% 19% .




- Molecule 35: 50S ribosomal protein L15

Chain RP:  79% 21% .




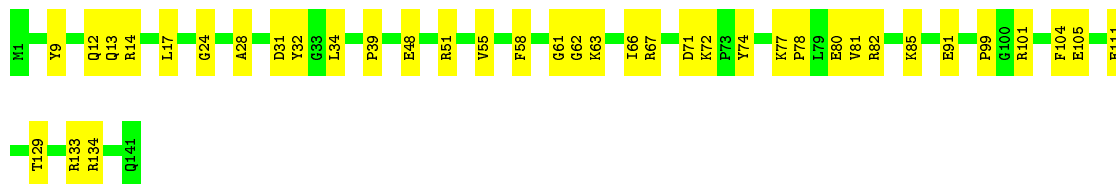
- Molecule 35: 50S ribosomal protein L15

Chain YP:  78% 19% ..




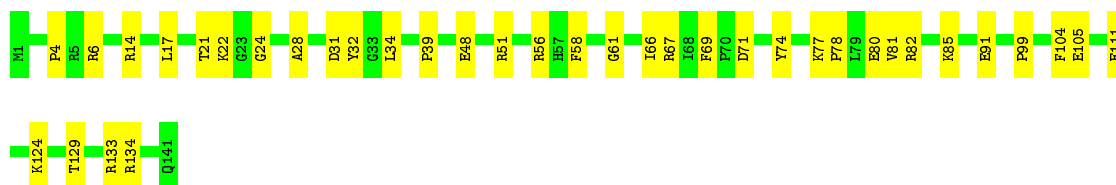
- Molecule 36: 50S ribosomal protein L16

Chain RQ:  73% 27%




- Molecule 36: 50S ribosomal protein L16

Chain YQ:  74% 26%




- Molecule 37: 50S ribosomal protein L17

Chain RR:  79% 20%




- Molecule 37: 50S ribosomal protein L17

Chain YR:  85% 14%




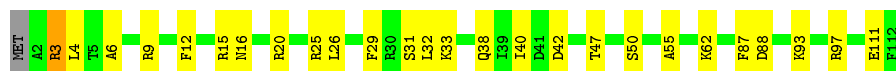
- Molecule 38: 50S ribosomal protein L18

Chain RS:  78% 21%



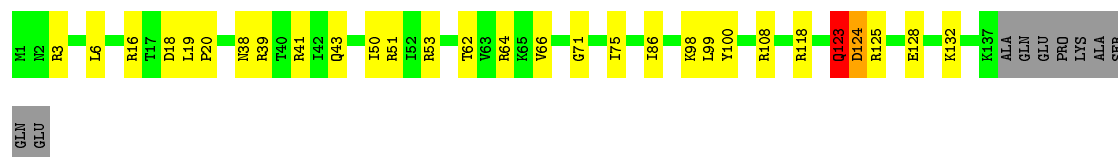
- Molecule 38: 50S ribosomal protein L18

Chain YS:  76% 22%



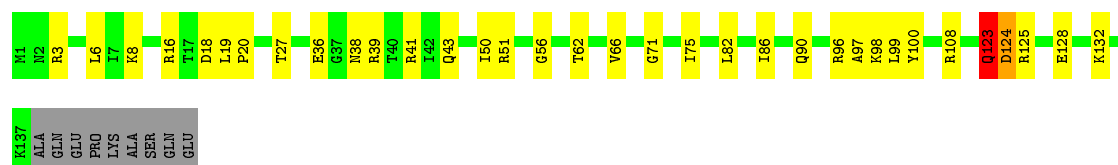
- Molecule 39: 50S ribosomal protein L19

Chain RT:  74% 18% 6%



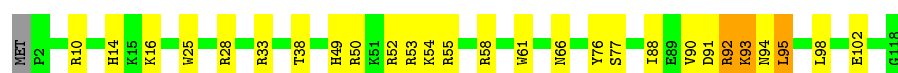
- Molecule 39: 50S ribosomal protein L19

Chain YT: 71% 22% 6%



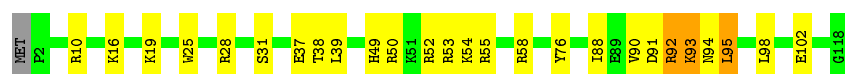
- Molecule 40: 50S ribosomal protein L20

Chain RU: 76% 20% 4%



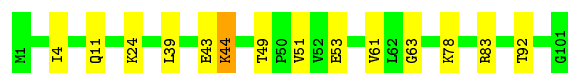
- Molecule 40: 50S ribosomal protein L20

Chain YU: 77% 19% 4%



- Molecule 41: 50S ribosomal protein L21

Chain RV: 86% 13% 1%



- Molecule 41: 50S ribosomal protein L21

Chain YV: 88% 10% 2%




- Molecule 42: 50S ribosomal protein L22

Chain RW: 84% 15% 1%



- Molecule 42: 50S ribosomal protein L22

Chain YW:  85% 15%



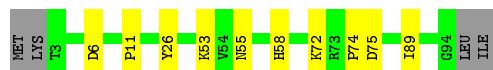
- Molecule 43: 50S ribosomal protein L23

Chain RX:  86% 9%




- Molecule 43: 50S ribosomal protein L23

Chain YX:  85% 10%




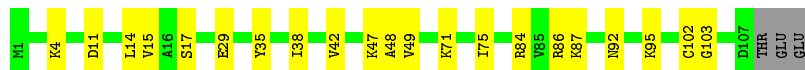
- Molecule 44: 50S ribosomal protein L24

Chain RY:  84% 14%



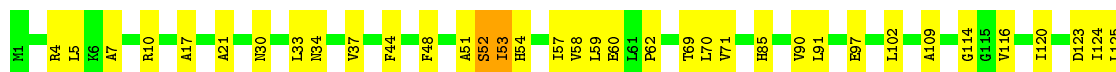
- Molecule 44: 50S ribosomal protein L24

Chain YY:  78% 19%




- Molecule 45: 50S ribosomal protein L25

Chain RZ:  66% 22% 11%



- Molecule 45: 50S ribosomal protein L25

Chain YZ:  66% 21% 11%

Chain R3:  85% 13%




- Molecule 49: 50S ribosomal protein L30

Chain Y3:  88% 10%




- Molecule 50: 50S ribosomal protein L31

Chain R4:  82% 13%




- Molecule 50: 50S ribosomal protein L31

Chain Y4:  77% 17%




- Molecule 51: 50S ribosomal protein L32

Chain R5:  85% 13%




- Molecule 51: 50S ribosomal protein L32

Chain Y5:  85% 13%




- Molecule 52: 50S ribosomal protein L33

Chain R6:  76% 22%




- Molecule 52: 50S ribosomal protein L33

Chain Y6:  80% 19%



- Molecule 53: 50S ribosomal protein L34

Chain R7:  84% 12%




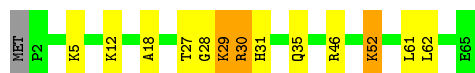
- Molecule 53: 50S ribosomal protein L34

Chain Y7:  86% 12%



- Molecule 54: 50S ribosomal protein L35

Chain R8:  78% 15% 5%




- Molecule 54: 50S ribosomal protein L35

Chain Y8:  80% 14% 5%




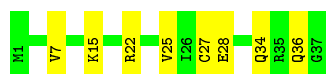
- Molecule 55: 50S ribosomal protein L36

Chain R9:  84% 16%



- Molecule 55: 50S ribosomal protein L36

Chain Y9:  78% 22%



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.81Å 448.83Å 618.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	134.68 – 3.74	Depositor
% Data completeness (in resolution range)	100.0 (134.68-3.74)	Depositor
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.58Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.204 , 0.225	Depositor
Wilson B-factor (Å ²)	112.7	Xtriage
Anisotropy	0.103	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	295646	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, SF4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	QA	0.96	0/36094	1.18	226/56334 (0.4%)
1	XA	0.96	0/36097	1.18	214/56339 (0.4%)
2	QB	0.40	0/1942	0.62	0/2619
2	XB	0.40	0/1950	0.59	0/2630
3	QC	0.39	0/1629	0.56	0/2195
3	XC	0.39	0/1629	0.56	0/2195
4	QD	0.45	0/1733	0.57	0/2318
4	XD	0.45	0/1733	0.57	0/2318
5	QE	0.42	0/1171	0.58	0/1576
5	XE	0.42	0/1171	0.58	0/1576
6	QF	0.44	0/856	0.58	0/1154
6	XF	0.44	0/856	0.58	0/1154
7	QG	0.36	0/1276	0.51	0/1709
7	XG	0.36	0/1276	0.51	0/1709
8	QH	0.44	0/1128	0.57	0/1517
8	XH	0.44	0/1128	0.56	0/1517
9	QI	0.44	0/1029	0.64	0/1379
9	XI	0.43	1/1017 (0.1%)	0.61	0/1365
10	QJ	0.42	0/814	0.62	1/1095 (0.1%)
10	XJ	0.40	0/790	0.61	1/1063 (0.1%)
11	QK	0.45	0/900	0.55	0/1213
11	XK	0.42	0/879	0.54	0/1187
12	QL	0.50	0/991	0.66	0/1327
12	XL	0.57	1/972 (0.1%)	0.68	0/1301
13	QM	0.41	0/965	0.62	0/1292
13	XM	0.39	0/956	0.61	0/1281
14	QN	0.51	0/501	0.60	0/664
14	XN	0.51	0/501	0.60	0/664
15	QO	0.40	0/745	0.55	0/992
15	XO	0.39	0/740	0.53	0/987
16	QP	0.49	0/721	0.58	0/970
16	XP	0.49	0/721	0.58	0/970

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	QQ	0.45	0/847	0.58	0/1131
17	XQ	0.45	0/847	0.58	0/1131
18	QR	0.39	0/579	0.62	0/768
18	XR	0.39	0/579	0.63	0/768
19	QS	0.38	0/680	0.71	1/915 (0.1%)
19	XS	0.40	0/689	0.66	0/926
20	QT	0.35	0/765	0.61	0/1007
20	XT	0.35	0/765	0.61	0/1007
21	QU	0.46	0/221	0.74	0/288
21	XU	0.46	0/221	0.74	0/288
22	QV	0.94	1/1836 (0.1%)	1.22	21/2859 (0.7%)
22	QW	0.31	0/1832	0.96	2/2855 (0.1%)
22	XV	0.94	1/1836 (0.1%)	1.22	21/2859 (0.7%)
22	XW	0.29	0/1832	0.94	2/2855 (0.1%)
23	QX	0.99	0/185	0.85	0/285
23	XX	1.03	1/257 (0.4%)	0.85	0/398
24	QY	0.78	0/404	1.11	0/627
24	XY	0.78	0/404	1.11	0/627
25	RA	1.12	5/69521 (0.0%)	1.24	583/108529 (0.5%)
25	YA	1.16	13/69543 (0.0%)	1.25	546/108563 (0.5%)
26	RB	0.81	0/2878	1.23	25/4490 (0.6%)
26	YB	0.81	0/2878	1.22	25/4490 (0.6%)
27	RD	0.60	0/2165	0.71	1/2919 (0.0%)
27	YD	0.60	0/2165	0.71	1/2919 (0.0%)
28	RE	0.52	0/1601	0.71	2/2160 (0.1%)
28	YE	0.52	0/1601	0.71	2/2160 (0.1%)
29	RF	0.58	0/1620	0.62	0/2194
29	YF	0.58	0/1620	0.62	0/2194
30	RG	0.40	0/1499	0.66	1/2016 (0.0%)
30	YG	0.40	0/1499	0.66	1/2016 (0.0%)
31	RH	0.41	0/1362	0.64	0/1841
31	YH	0.41	0/1362	0.64	0/1841
32	RI	0.37	0/1151	0.65	0/1558
32	YI	0.37	0/1151	0.65	0/1558
33	RN	0.50	0/1131	0.64	0/1525
33	YN	0.50	0/1131	0.64	0/1525
34	RO	0.55	0/943	0.61	0/1269
34	YO	0.55	0/943	0.61	0/1269
35	RP	0.47	0/1162	0.76	1/1544 (0.1%)
35	YP	0.49	0/1139	0.76	1/1514 (0.1%)
36	RQ	0.48	0/1143	0.66	0/1527
36	YQ	0.48	0/1143	0.66	0/1527
37	RR	0.49	0/974	0.69	1/1302 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	YR	0.50	0/974	0.66	1/1302 (0.1%)
38	RS	0.38	0/892	0.70	0/1187
38	YS	0.38	0/892	0.70	0/1187
39	RT	0.46	0/1155	0.66	0/1542
39	YT	0.46	0/1155	0.66	0/1542
40	RU	0.52	0/982	0.61	0/1306
40	YU	0.52	0/982	0.61	0/1306
41	RV	0.47	0/790	0.67	0/1057
41	YV	0.46	0/790	0.67	0/1057
42	RW	0.54	0/911	0.61	0/1220
42	YW	0.55	0/911	0.61	0/1220
43	RX	0.56	0/739	0.58	0/993
43	YX	0.56	0/739	0.58	0/993
44	RY	0.53	0/831	0.56	0/1108
44	YY	0.53	0/831	0.56	0/1108
45	RZ	0.39	0/1493	0.71	0/2026
45	YZ	0.39	0/1493	0.71	0/2026
46	R0	0.51	0/652	0.57	0/867
46	Y0	0.47	0/607	0.56	0/809
47	R1	0.58	1/770 (0.1%)	0.64	0/1022
47	Y1	0.56	0/736	0.65	0/978
48	R2	0.40	0/583	0.52	0/771
48	Y2	0.40	0/583	0.52	0/771
49	R3	0.44	0/474	0.60	0/635
49	Y3	0.44	0/474	0.60	0/635
50	R4	0.37	0/578	0.64	0/776
50	Y4	0.37	0/578	0.64	0/776
51	R5	0.50	0/473	0.58	0/639
51	Y5	0.50	0/473	0.58	0/639
52	R6	0.34	0/460	0.51	0/613
52	Y6	0.34	0/460	0.51	0/613
53	R7	0.52	0/417	0.59	0/550
53	Y7	0.60	0/426	0.62	0/561
54	R8	0.55	0/525	0.76	0/691
54	Y8	0.55	0/525	0.76	0/691
55	R9	0.44	0/310	0.50	0/407
55	Y9	0.43	0/310	0.50	0/407
All	All	0.93	24/319989 (0.0%)	1.10	1680/478685 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	QB	0	1
4	QD	0	1
4	XD	0	1
12	QL	0	2
12	XL	0	2
13	QM	0	1
27	RD	0	4
27	YD	0	4
28	RE	0	3
28	YE	0	3
30	RG	0	1
30	YG	0	1
31	RH	0	1
31	YH	0	1
32	RI	0	3
32	YI	0	3
35	RP	0	1
35	YP	0	1
37	RR	0	1
39	RT	0	1
39	YT	0	1
40	RU	0	2
40	YU	0	2
41	RV	0	2
41	YV	0	2
45	RZ	0	4
45	YZ	0	4
50	R4	0	1
50	Y4	0	1
54	R8	0	4
54	Y8	0	4
All	All	0	63

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	XV	1	C	OP3-P	-10.70	1.48	1.61
22	QV	1	C	OP3-P	-10.69	1.48	1.61
25	YA	74	A	N9-C4	-6.89	1.33	1.37
25	RA	74	A	N9-C4	-6.79	1.33	1.37
23	XX	21	C	O3'-P	-6.62	1.53	1.61

The worst 5 of 1680 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	1158	C	C2-N1-C1'	13.01	133.12	118.80
1	QA	1301	U	N1-C2-O2	12.90	131.83	122.80
1	XA	1158	C	N1-C2-O2	12.82	126.59	118.90
1	QA	328	C	N1-C2-O2	12.57	126.44	118.90
1	QA	1301	U	N3-C2-O2	-12.21	113.65	122.20

There are no chirality outliers.

5 of 63 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	QB	15	VAL	Peptide
4	QD	19	LEU	Peptide
12	QL	104	VAL	Peptide
12	QL	47	LYS	Peptide
13	QM	66	LEU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32244	0	16274	320	0
1	XA	32246	0	16277	343	1
2	QB	1907	0	1958	36	0
2	XB	1915	0	1969	25	0
3	QC	1605	0	1668	17	0
3	XC	1605	0	1668	15	0
4	QD	1703	0	1766	30	0
4	XD	1703	0	1767	29	0
5	QE	1155	0	1213	12	0
5	XE	1155	0	1213	12	0
6	QF	843	0	857	12	0
6	XF	843	0	857	10	0
7	QG	1257	0	1296	18	0
7	XG	1257	0	1296	26	0
8	QH	1108	0	1165	14	0
8	XH	1108	0	1165	15	0
9	QI	1010	0	1037	24	0
9	XI	998	0	1024	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	QJ	801	0	849	17	0
10	XJ	777	0	816	16	0
11	QK	885	0	904	23	0
11	XK	864	0	881	23	0
12	QL	975	0	1062	16	0
12	XL	956	0	1046	18	0
13	QM	955	0	1021	19	0
13	XM	946	0	1007	20	0
14	QN	492	0	529	8	0
14	XN	492	0	529	7	0
15	QO	734	0	771	4	0
15	XO	729	0	768	8	0
16	QP	705	0	725	11	0
16	XP	705	0	725	9	0
17	QQ	834	0	904	14	0
17	XQ	834	0	904	17	0
18	QR	574	0	644	8	0
18	XR	574	0	644	6	0
19	QS	665	0	686	13	0
19	XS	674	0	699	9	0
20	QT	763	0	860	9	0
20	XT	763	0	861	11	0
21	QU	217	0	234	8	0
21	XU	217	0	234	8	0
22	QV	1644	0	836	10	0
22	QW	1640	0	837	57	0
22	XV	1644	0	836	9	0
22	XW	1640	0	837	71	0
23	QX	167	0	86	3	0
23	XX	230	0	120	17	0
24	QY	362	0	183	3	0
24	XY	362	0	184	3	0
25	RA	62071	0	31285	461	0
25	YA	62091	0	31290	472	1
26	RB	2573	0	1306	26	0
26	YB	2573	0	1306	28	1
27	RD	2115	0	2195	49	0
27	YD	2115	0	2195	48	0
28	RE	1568	0	1634	29	0
28	YE	1568	0	1634	33	0
29	RF	1585	0	1632	24	0
29	YF	1585	0	1632	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	RG	1474	0	1535	26	0
30	YG	1474	0	1535	32	0
31	RH	1336	0	1418	19	0
31	YH	1336	0	1418	20	0
32	RI	1136	0	1223	12	1
32	YI	1136	0	1223	14	0
33	RN	1104	0	1180	9	0
33	YN	1104	0	1180	8	0
34	RO	933	0	996	20	0
34	YO	933	0	996	19	0
35	RP	1145	0	1227	25	0
35	YP	1122	0	1204	25	0
36	RQ	1122	0	1179	31	0
36	YQ	1122	0	1179	24	0
37	RR	960	0	1021	14	0
37	YR	960	0	1021	9	0
38	RS	882	0	943	18	0
38	YS	882	0	943	20	0
39	RT	1141	0	1202	23	0
39	YT	1141	0	1202	25	0
40	RU	964	0	1022	33	0
40	YU	964	0	1022	24	0
41	RV	779	0	852	9	0
41	YV	779	0	852	7	4
42	RW	900	0	964	13	1
42	YW	900	0	964	12	0
43	RX	725	0	778	6	0
43	YX	725	0	778	7	0
44	RY	818	0	909	8	4
44	YY	818	0	909	15	1
45	RZ	1461	0	1493	28	0
45	YZ	1461	0	1493	26	0
46	R0	643	0	667	10	0
46	Y0	599	0	617	13	0
47	R1	763	0	848	14	0
47	Y1	729	0	802	10	0
48	R2	581	0	629	9	0
48	Y2	581	0	629	11	4
49	R3	469	0	518	6	0
49	Y3	469	0	518	3	0
50	R4	565	0	557	8	0
50	Y4	565	0	557	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	R5	459	0	476	6	0
51	Y5	459	0	479	4	4
52	R6	453	0	473	8	0
52	Y6	453	0	473	6	0
53	R7	409	0	454	4	0
53	Y7	418	0	467	5	0
54	R8	517	0	582	14	0
54	Y8	517	0	582	10	0
55	R9	307	0	335	4	0
55	Y9	307	0	335	6	0
56	QA	72	0	0	0	0
56	QC	1	0	0	0	0
56	QF	1	0	0	0	0
56	QH	1	0	0	0	0
56	QV	6	0	0	0	0
56	QX	1	0	0	0	0
56	QY	1	0	0	0	0
56	R0	3	0	0	0	0
56	R8	1	0	0	0	0
56	RA	513	0	0	0	0
56	RB	11	0	0	0	0
56	RE	3	0	0	0	0
56	RN	1	0	0	0	0
56	RO	1	0	0	0	0
56	RP	2	0	0	0	0
56	RQ	2	0	0	0	0
56	RR	2	0	0	0	0
56	RT	1	0	0	0	0
56	RY	1	0	0	0	0
56	XA	80	0	0	0	0
56	XC	1	0	0	0	0
56	XE	1	0	0	0	0
56	XL	1	0	0	0	0
56	XM	1	0	0	0	0
56	XQ	1	0	0	0	0
56	XS	1	0	0	0	0
56	XV	8	0	0	0	0
56	XX	1	0	0	0	0
56	Y0	2	0	0	0	0
56	Y5	1	0	0	0	0
56	Y7	1	0	0	0	0
56	Y8	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	YA	541	0	0	0	0
56	YB	12	0	0	0	0
56	YD	1	0	0	0	0
56	YE	3	0	0	0	0
56	YO	1	0	0	0	0
56	YP	4	0	0	0	0
56	YQ	3	0	0	0	0
56	YX	2	0	0	0	0
56	YY	1	0	0	0	0
57	QD	8	0	0	0	0
57	XD	8	0	0	0	0
58	QN	1	0	0	0	0
58	R4	1	0	0	0	0
58	R5	1	0	0	0	0
58	R6	1	0	0	0	0
58	R9	1	0	0	0	0
58	RY	1	0	0	0	0
58	XN	1	0	0	0	0
58	Y4	1	0	0	0	0
58	Y5	1	0	0	0	0
58	Y6	1	0	0	0	0
58	Y9	1	0	0	0	0
58	YY	1	0	0	0	0
All	All	295646	0	199660	2768	11

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 2768 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:XG:143:ARG:CD	22:XW:42:C:O3'	1.75	1.33
7:QG:143:ARG:HD3	22:QW:42:C:O3'	1.09	1.24
7:QG:143:ARG:CD	22:QW:42:C:O3'	1.88	1.20
23:XX:22:C:H6	23:XX:22:C:H5''	1.06	1.13
11:XK:54:ARG:HH22	22:XW:40:C:H4'	1.12	1.09

The worst 5 of 11 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:YA:1411:C:O2'	26:YB:53:A:O2'[1_655]	1.11	1.09
41:YV:49:THR:O	51:Y5:59:GLU:OE2[4_445]	1.56	0.64
44:RY:21:LYS:NZ	48:Y2:71:ASN:CB[3_555]	1.64	0.56
44:RY:19:LYS:O	48:Y2:71:ASN:ND2[3_555]	1.71	0.49
41:YV:49:THR:OG1	51:Y5:60:VAL:O[4_445]	1.86	0.34

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QB	233/256 (91%)	207 (89%)	25 (11%)	1 (0%)	34	69
2	XB	234/256 (91%)	208 (89%)	26 (11%)	0	100	100
3	QC	203/239 (85%)	188 (93%)	15 (7%)	0	100	100
3	XC	203/239 (85%)	188 (93%)	15 (7%)	0	100	100
4	QD	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
4	XD	206/209 (99%)	190 (92%)	16 (8%)	0	100	100
5	QE	149/162 (92%)	144 (97%)	4 (3%)	1 (1%)	22	59
5	XE	149/162 (92%)	144 (97%)	4 (3%)	1 (1%)	22	59
6	QF	99/101 (98%)	99 (100%)	0	0	100	100
6	XF	99/101 (98%)	99 (100%)	0	0	100	100
7	QG	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
7	XG	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
8	QH	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
8	XH	135/138 (98%)	128 (95%)	7 (5%)	0	100	100
9	QI	125/128 (98%)	115 (92%)	10 (8%)	0	100	100
9	XI	124/128 (97%)	114 (92%)	10 (8%)	0	100	100
10	QJ	97/105 (92%)	87 (90%)	10 (10%)	0	100	100
10	XJ	94/105 (90%)	83 (88%)	11 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	QK	117/129 (91%)	106 (91%)	11 (9%)	0	100	100
11	XK	114/129 (88%)	109 (96%)	5 (4%)	0	100	100
12	QL	123/132 (93%)	106 (86%)	17 (14%)	0	100	100
12	XL	120/132 (91%)	106 (88%)	13 (11%)	1 (1%)	19	56
13	QM	118/126 (94%)	99 (84%)	18 (15%)	1 (1%)	19	56
13	XM	117/126 (93%)	98 (84%)	19 (16%)	0	100	100
14	QN	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	9	43
14	XN	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	9	43
15	QO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
15	XO	85/89 (96%)	85 (100%)	0	0	100	100
16	QP	82/88 (93%)	80 (98%)	2 (2%)	0	100	100
16	XP	82/88 (93%)	80 (98%)	2 (2%)	0	100	100
17	QQ	98/105 (93%)	95 (97%)	3 (3%)	0	100	100
17	XQ	98/105 (93%)	95 (97%)	3 (3%)	0	100	100
18	QR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
18	XR	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
19	QS	81/93 (87%)	69 (85%)	12 (15%)	0	100	100
19	XS	82/93 (88%)	67 (82%)	15 (18%)	0	100	100
20	QT	97/106 (92%)	86 (89%)	11 (11%)	0	100	100
20	XT	97/106 (92%)	86 (89%)	11 (11%)	0	100	100
21	QU	23/27 (85%)	20 (87%)	3 (13%)	0	100	100
21	XU	23/27 (85%)	20 (87%)	3 (13%)	0	100	100
27	RD	270/276 (98%)	247 (92%)	22 (8%)	1 (0%)	34	69
27	YD	270/276 (98%)	247 (92%)	22 (8%)	1 (0%)	34	69
28	RE	203/206 (98%)	165 (81%)	36 (18%)	2 (1%)	15	51
28	YE	203/206 (98%)	165 (81%)	36 (18%)	2 (1%)	15	51
29	RF	200/210 (95%)	181 (90%)	19 (10%)	0	100	100
29	YF	200/210 (95%)	181 (90%)	19 (10%)	0	100	100
30	RG	179/182 (98%)	148 (83%)	30 (17%)	1 (1%)	25	61
30	YG	179/182 (98%)	148 (83%)	30 (17%)	1 (1%)	25	61
31	RH	172/180 (96%)	151 (88%)	17 (10%)	4 (2%)	6	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	YH	172/180 (96%)	151 (88%)	17 (10%)	4 (2%)	6	38
32	RI	144/148 (97%)	124 (86%)	18 (12%)	2 (1%)	11	46
32	YI	144/148 (97%)	124 (86%)	18 (12%)	2 (1%)	11	46
33	RN	136/140 (97%)	119 (88%)	16 (12%)	1 (1%)	22	59
33	YN	136/140 (97%)	119 (88%)	16 (12%)	1 (1%)	22	59
34	RO	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
34	YO	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
35	RP	148/150 (99%)	117 (79%)	30 (20%)	1 (1%)	22	59
35	YP	145/150 (97%)	113 (78%)	31 (21%)	1 (1%)	22	59
36	RQ	139/141 (99%)	114 (82%)	24 (17%)	1 (1%)	22	59
36	YQ	139/141 (99%)	114 (82%)	24 (17%)	1 (1%)	22	59
37	RR	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17	53
37	YR	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17	53
38	RS	109/112 (97%)	93 (85%)	16 (15%)	0	100	100
38	YS	109/112 (97%)	93 (85%)	16 (15%)	0	100	100
39	RT	135/146 (92%)	119 (88%)	14 (10%)	2 (2%)	10	45
39	YT	135/146 (92%)	119 (88%)	14 (10%)	2 (2%)	10	45
40	RU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17	53
40	YU	115/118 (98%)	107 (93%)	7 (6%)	1 (1%)	17	53
41	RV	99/101 (98%)	89 (90%)	10 (10%)	0	100	100
41	YV	99/101 (98%)	89 (90%)	10 (10%)	0	100	100
42	RW	111/113 (98%)	102 (92%)	9 (8%)	0	100	100
42	YW	111/113 (98%)	102 (92%)	9 (8%)	0	100	100
43	RX	90/96 (94%)	87 (97%)	3 (3%)	0	100	100
43	YX	90/96 (94%)	87 (97%)	3 (3%)	0	100	100
44	RY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
44	YY	105/110 (96%)	101 (96%)	4 (4%)	0	100	100
45	RZ	181/206 (88%)	150 (83%)	29 (16%)	2 (1%)	14	50
45	YZ	181/206 (88%)	149 (82%)	30 (17%)	2 (1%)	14	50
46	R0	79/85 (93%)	74 (94%)	5 (6%)	0	100	100
46	Y0	73/85 (86%)	67 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	R1	95/98 (97%)	83 (87%)	12 (13%)	0	100	100
47	Y1	91/98 (93%)	77 (85%)	14 (15%)	0	100	100
48	R2	67/72 (93%)	64 (96%)	2 (3%)	1 (2%)	10	45
48	Y2	67/72 (93%)	64 (96%)	2 (3%)	1 (2%)	10	45
49	R3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
49	Y3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
50	R4	67/71 (94%)	55 (82%)	11 (16%)	1 (2%)	10	45
50	Y4	67/71 (94%)	55 (82%)	11 (16%)	1 (2%)	10	45
51	R5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
51	Y5	57/60 (95%)	55 (96%)	2 (4%)	0	100	100
52	R6	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
52	Y6	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
53	R7	45/49 (92%)	45 (100%)	0	0	100	100
53	Y7	46/49 (94%)	46 (100%)	0	0	100	100
54	R8	62/65 (95%)	47 (76%)	13 (21%)	2 (3%)	4	32
54	Y8	62/65 (95%)	47 (76%)	13 (21%)	2 (3%)	4	32
55	R9	35/37 (95%)	35 (100%)	0	0	100	100
55	Y9	35/37 (95%)	35 (100%)	0	0	100	100
All	All	11452/12128 (94%)	10311 (90%)	1088 (10%)	53 (0%)	29	65

5 of 53 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
39	RT	124	ASP
45	RZ	53	ILE
39	YT	124	ASP
45	YZ	53	ILE
14	QN	17	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	QB	203/220 (92%)	202 (100%)	1 (0%)	88	94
2	XB	204/220 (93%)	201 (98%)	3 (2%)	65	81
3	QC	159/188 (85%)	158 (99%)	1 (1%)	86	92
3	XC	159/188 (85%)	158 (99%)	1 (1%)	86	92
4	QD	180/181 (99%)	179 (99%)	1 (1%)	86	92
4	XD	180/181 (99%)	179 (99%)	1 (1%)	86	92
5	QE	116/123 (94%)	115 (99%)	1 (1%)	78	88
5	XE	116/123 (94%)	115 (99%)	1 (1%)	78	88
6	QF	90/90 (100%)	89 (99%)	1 (1%)	73	85
6	XF	90/90 (100%)	89 (99%)	1 (1%)	73	85
7	QG	126/127 (99%)	126 (100%)	0	100	100
7	XG	126/127 (99%)	126 (100%)	0	100	100
8	QH	118/119 (99%)	118 (100%)	0	100	100
8	XH	118/119 (99%)	118 (100%)	0	100	100
9	QI	98/99 (99%)	96 (98%)	2 (2%)	55	75
9	XI	97/99 (98%)	97 (100%)	0	100	100
10	QJ	89/92 (97%)	89 (100%)	0	100	100
10	XJ	86/92 (94%)	86 (100%)	0	100	100
11	QK	90/99 (91%)	90 (100%)	0	100	100
11	XK	88/99 (89%)	88 (100%)	0	100	100
12	QL	104/109 (95%)	104 (100%)	0	100	100
12	XL	103/109 (94%)	103 (100%)	0	100	100
13	QM	96/101 (95%)	96 (100%)	0	100	100
13	XM	95/101 (94%)	95 (100%)	0	100	100
14	QN	49/50 (98%)	48 (98%)	1 (2%)	55	75
14	XN	49/50 (98%)	48 (98%)	1 (2%)	55	75
15	QO	79/80 (99%)	79 (100%)	0	100	100
15	XO	79/80 (99%)	79 (100%)	0	100	100
16	QP	72/74 (97%)	71 (99%)	1 (1%)	67	82
16	XP	72/74 (97%)	71 (99%)	1 (1%)	67	82
17	QQ	95/97 (98%)	95 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	XQ	95/97 (98%)	95 (100%)	0	100	100
18	QR	61/77 (79%)	61 (100%)	0	100	100
18	XR	61/77 (79%)	61 (100%)	0	100	100
19	QS	72/80 (90%)	71 (99%)	1 (1%)	67	82
19	XS	73/80 (91%)	72 (99%)	1 (1%)	67	82
20	QT	76/82 (93%)	76 (100%)	0	100	100
20	XT	76/82 (93%)	76 (100%)	0	100	100
21	QU	20/22 (91%)	20 (100%)	0	100	100
21	XU	20/22 (91%)	20 (100%)	0	100	100
27	RD	214/218 (98%)	212 (99%)	2 (1%)	78	88
27	YD	214/218 (98%)	212 (99%)	2 (1%)	78	88
28	RE	165/166 (99%)	165 (100%)	0	100	100
28	YE	165/166 (99%)	165 (100%)	0	100	100
29	RF	161/166 (97%)	159 (99%)	2 (1%)	71	84
29	YF	161/166 (97%)	159 (99%)	2 (1%)	71	84
30	RG	155/156 (99%)	153 (99%)	2 (1%)	69	82
30	YG	155/156 (99%)	153 (99%)	2 (1%)	69	82
31	RH	145/148 (98%)	141 (97%)	4 (3%)	43	67
31	YH	145/148 (98%)	141 (97%)	4 (3%)	43	67
32	RI	122/124 (98%)	122 (100%)	0	100	100
32	YI	122/124 (98%)	122 (100%)	0	100	100
33	RN	117/119 (98%)	116 (99%)	1 (1%)	78	88
33	YN	117/119 (98%)	116 (99%)	1 (1%)	78	88
34	RO	100/100 (100%)	98 (98%)	2 (2%)	55	75
34	YO	100/100 (100%)	98 (98%)	2 (2%)	55	75
35	RP	116/116 (100%)	114 (98%)	2 (2%)	60	79
35	YP	114/116 (98%)	113 (99%)	1 (1%)	78	88
36	RQ	111/111 (100%)	111 (100%)	0	100	100
36	YQ	111/111 (100%)	111 (100%)	0	100	100
37	RR	100/101 (99%)	100 (100%)	0	100	100
37	YR	100/101 (99%)	100 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	RS	87/88 (99%)	86 (99%)	1 (1%)	73	85
38	YS	87/88 (99%)	86 (99%)	1 (1%)	73	85
39	RT	120/127 (94%)	119 (99%)	1 (1%)	81	89
39	YT	120/127 (94%)	119 (99%)	1 (1%)	81	89
40	RU	93/94 (99%)	93 (100%)	0	100	100
40	YU	93/94 (99%)	93 (100%)	0	100	100
41	RV	82/82 (100%)	82 (100%)	0	100	100
41	YV	82/82 (100%)	82 (100%)	0	100	100
42	RW	92/92 (100%)	90 (98%)	2 (2%)	52	72
42	YW	92/92 (100%)	90 (98%)	2 (2%)	52	72
43	RX	74/78 (95%)	74 (100%)	0	100	100
43	YX	74/78 (95%)	74 (100%)	0	100	100
44	RY	88/91 (97%)	88 (100%)	0	100	100
44	YY	88/91 (97%)	88 (100%)	0	100	100
45	RZ	162/179 (90%)	161 (99%)	1 (1%)	86	92
45	YZ	162/179 (90%)	161 (99%)	1 (1%)	86	92
46	R0	65/67 (97%)	64 (98%)	1 (2%)	65	81
46	Y0	61/67 (91%)	60 (98%)	1 (2%)	62	79
47	R1	82/83 (99%)	82 (100%)	0	100	100
47	Y1	78/83 (94%)	78 (100%)	0	100	100
48	R2	64/67 (96%)	64 (100%)	0	100	100
48	Y2	64/67 (96%)	64 (100%)	0	100	100
49	R3	51/52 (98%)	50 (98%)	1 (2%)	55	75
49	Y3	51/52 (98%)	50 (98%)	1 (2%)	55	75
50	R4	62/63 (98%)	61 (98%)	1 (2%)	62	79
50	Y4	62/63 (98%)	61 (98%)	1 (2%)	62	79
51	R5	51/52 (98%)	51 (100%)	0	100	100
51	Y5	51/52 (98%)	51 (100%)	0	100	100
52	R6	51/52 (98%)	51 (100%)	0	100	100
52	Y6	51/52 (98%)	51 (100%)	0	100	100
53	R7	40/42 (95%)	40 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	Y7	41/42 (98%)	41 (100%)	0	100	100
54	R8	54/55 (98%)	54 (100%)	0	100	100
54	Y8	54/55 (98%)	54 (100%)	0	100	100
55	R9	34/34 (100%)	34 (100%)	0	100	100
55	Y9	34/34 (100%)	34 (100%)	0	100	100
All	All	9687/10066 (96%)	9622 (99%)	65 (1%)	84	91

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	RZ	34	ASN
3	XC	165	THR
42	YW	40	ASN
46	R0	14	ARG
2	XB	30	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
45	RZ	32	HIS
2	XB	40	HIS
43	YX	41	ASN
48	R2	46	GLN
5	XE	73	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1498/1508 (99%)	297 (19%)	32 (2%)
1	XA	1498/1508 (99%)	282 (18%)	27 (1%)
22	QV	76/77 (98%)	15 (19%)	2 (2%)
22	QW	76/77 (98%)	33 (43%)	2 (2%)
22	XV	76/77 (98%)	15 (19%)	2 (2%)
22	XW	76/77 (98%)	34 (44%)	2 (2%)
23	QX	7/25 (28%)	0	0
23	XX	10/25 (40%)	2 (20%)	0
24	QY	16/17 (94%)	4 (25%)	0
24	XY	16/17 (94%)	4 (25%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
25	RA	2879/2915 (98%)	613 (21%)	41 (1%)
25	YA	2880/2915 (98%)	609 (21%)	41 (1%)
26	RB	119/122 (97%)	24 (20%)	0
26	YB	119/122 (97%)	24 (20%)	0
All	All	9346/9482 (98%)	1956 (20%)	149 (1%)

5 of 1956 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	6	G
1	QA	32	A
1	QA	39	G
1	QA	41	G
1	QA	47	C

5 of 149 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	RA	1992	G
1	XA	243	A
25	YA	1819	A
25	RA	2210	G
25	RA	2776	A

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1306 ligands modelled in this entry, 1304 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
57	SF4	QD	301	4	0,12,12	0.00	-	-		
57	SF4	XD	301	4	0,12,12	0.00	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	SF4	QD	301	4	-	-	0/6/5/5
57	SF4	XD	301	4	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.